Chapter 6

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TIME-MARCHING METHODS FOR ODE'S

- Discretization of spatial derivatives in the governing PDE's (e.g., the Navier-Stokes equations)
  - Leads to coupled system of nonlinear ODE's in the form

$$\frac{d\vec{u}}{dt} = \vec{F}(\vec{u}, t) \tag{1}$$

  - Can be integrated in time using a time-marching method to obtain a time-accurate solution to an *unsteady* flow problem.
  - For a *steady* flow problem, spatial discretization leads to a coupled system of nonlinear algebraic equations in the form

$$\vec{F}(\vec{u}) = 0 \tag{2}$$

- Nonlinearity leads to iterative methods to obtain solutions.

- Linearization will produce coupled systems of linear algebraic equations which must be solved at each iteration.
- These can be solved iteratively using relaxation methods
- Alternatively, a time-dependent path to the steady state
- Time-marching method to integrate the unsteady equations
  - To accurately resolve on unsteady solution in time.
  - Until the solution is sufficiently close to the steady solution.
- When using a time-marching method to compute steady flows
  - The goal is simply to remove the transient portion of the solution as quickly as possible
  - Time-accuracy is not required.
  - This motivates the study of stability and stiffness.

Notation

- Using the semi-discrete approach
- Reduce PDE to a set of coupled ODE's
- Consider the scalar case

$$\frac{du}{dt} = u' = F(u,t) \tag{3}$$

- Subscript n, $h = \Delta t$, gives

$$u'_n = F_n = F(u_n, t_n) \quad , \quad t_n = nh$$

- Intermediate time steps involving temporary calculations $\tilde{u}$, $\bar{u}$, etc.

$$\tilde{u}'_{n+\alpha} = \tilde{F}_{n+\alpha} = F(\tilde{u}_{n+\alpha}, t_n + \alpha h)$$

Converting Time-Marching Methods to $O\Delta E$'s

Three representative examples of $O\Delta E$'s

$$u_{n+1} = u_n + hu'_n \quad \textit{Euler Explicit} \tag{4}$$

$$u_{n+1} = u_n + hu'_{n+1} \quad \textit{Euler Implicit} \tag{5}$$

Predictor-Corrector

$$\begin{aligned} \tilde{u}_{n+1} &= u_n + hu'_n && \textit{Predictor} \\ u_{n+1} &= \frac{1}{2}[u_n + \tilde{u}_{n+1} + h\tilde{u}'_{n+1}] && \textit{Corrector} \end{aligned} \tag{6}$$

Converting Time-Marching Methods to $O\Delta E$'s

- Representative ODE:

$$\frac{du}{dt} = u' = \lambda u + ae^{\mu t} \tag{7}$$

- Replacing u' in Eq.' 4 $\quad u_{n+1} = u_n + hu'_n$

$$u_{n+1} = u_n + h(\lambda u_n + ae^{\mu hn}) \quad or$$

$$u_{n+1} - (1 + \lambda h)u_n = hae^{\mu hn} \tag{8}$$

- Implicit Euler method, Eq. 5, $\quad u_{n+1} = u_n + hu'_{n+1}$

$$u_{n+1} = u_n + h\left(\lambda u_{n+1} + ae^{\mu h(n+1)}\right) \quad or$$

$$(1 - \lambda h)u_{n+1} - u_n = he^{\mu h} \cdot ae^{\mu hn} \tag{9}$$

- The predictor-corrector sequence, Eq. 6, gives

$$
\begin{aligned}
\tilde{u}_{n+1} - (1+\lambda h)u_n &= ahe^{\mu hn} \\
-\frac{1}{2}(1+\lambda h)\tilde{u}_{n+1} + u_{n+1} - \frac{1}{2}u_n &= \frac{1}{2}ahe^{\mu h(n+1)}
\end{aligned}
\tag{10}
$$

- **Coupled** set of linear OΔE's with constant coefficients.

- First line of Eq. 10 Predictor step: explicit Euler method.

- The second line Corrector step: note that

$$
\begin{aligned}
\tilde{u}'_{n+1} &= F(\tilde{u}_{n+1}, t_n + h) \\
&= \lambda\tilde{u}_{n+1} + ae^{\mu h(n+1)}
\end{aligned}
$$

Euler Explicit: Recursive Solution

- Using Eq.8 with $a = 0$ (simplifies analysis)

$$u_{n+1} = (1 + \lambda h)u_n$$

- Let u_0, time $t = 0, n = 0$ be initial condition (IC)
- Then

$$\begin{aligned} u_1 &= (1 + \lambda h)u_0 \\ u_2 = (1 + \lambda h)u_1 &= (1 + \lambda h)^2 u_0 \\ u_3 = (1 + \lambda h)u_2 &= (1 + \lambda h)^3 u_0 \\ &\vdots \\ u_n &= (1 + \lambda h)^n u_0 \end{aligned} \tag{11}$$

Euler Implicit: Recursive Solution

- Using Eq.9 with $a = 0$ (simplifies analysis)

$$u_{n+1} = \left(\frac{1}{1-\lambda h}\right) u_n$$

- Then

$$\begin{aligned} u_1 &= \left(\frac{1}{1-\lambda h}\right) u_0 \\ u_2 = \left(\frac{1}{1-\lambda h}\right) u_1 &= \left(\frac{1}{1-\lambda h}\right)^2 u_0 \\ &\vdots \\ u_n &= \left(\frac{1}{1-\lambda h}\right)^n u_0 \end{aligned} \tag{12}$$

Predictor- Corrector: Recursive Solution

- Using Eq.10 with $a = 0$

$$\tilde{u}_{n+1} = (1 + \lambda h)u_n \quad : \textit{Predictor Step} \tag{13}$$

$$u_{n+1} = \frac{1}{2}\left(u_n + \tilde{u}_{n+1} + \lambda h \tilde{u}_{n+1}\right) \quad : \textit{Corrector Step} \tag{14}$$

- Substituting Eq.13 into Eq.14

$$u_{n+1} = \left(1 + \lambda h + \frac{1}{2}(\lambda h)^2\right) u_n$$

- By recursion

$$u_{n+1} = \left(1 + \lambda h + \frac{1}{2}(\lambda h)^2\right)^n u_0 \tag{15}$$

Recursive Solution with Forcing Function

- Using Eq.8 with $a \neq 0$

$$u_{n+1} = (1+\lambda h)u_n + ae^{\mu h n}$$

$$\begin{aligned}
u_1 &= (1+\lambda h)u_0 + a \\
u_2 &= (1+\lambda h)u_1 + ae^{\mu h} = \\
&\quad (1+\lambda h)\left((1+\lambda h)u_0 + a\right) + ae^{\mu h} = \\
&\quad (1+\lambda h)^2 u_0 + (1+\lambda h)a\left(1+e^{\mu h}\right) \\
&\vdots \\
u_n &= (1+\lambda h)^n u_0 + \sum_{l=1}^{n}(1+\lambda h)^{l-1} a e^{(l-1)\mu h} \qquad (16)
\end{aligned}$$

Generalize Solutions, $O\Delta E$

- Recursive solutions in general are difficult and complicated
- There is a generalize procedure for $O\Delta E$'s
- Note the general form of the solutions, Eq.11,12, and 15

$$u_n = \sigma^n u_0$$

with

$$\begin{aligned}
\sigma_{ee} &= (1 + \lambda h) \\
\sigma_{ei} &= \left(\frac{1}{1 - \lambda h} \right) \\
\sigma_{pc} &= \left(1 + \lambda h + \frac{1}{2} (\lambda h)^2 \right)
\end{aligned}$$

Notation and Displacement Operator

- $O\Delta E$ difference displacement operator, E

$$u_{n+1} = Eu_n \quad , \quad u_{n+k} = E^k u_n$$

- The displacement operator also applies to exponents, thus

$$b^\alpha \cdot b^n = b^{n+\alpha} = E^\alpha \cdot b^n$$

where α can be any fraction or irrational number.

- For example:

$$u_{n+2} = E^2 u_n, \quad u_{n+\frac{1}{5}} = E^{\frac{1}{5}} u_n$$

$$e^{\mu h(n+3)} = E^3 e^{\mu h(n)} \quad e^{\mu h(n-\frac{2}{3})} = E^{-\frac{2}{3}} e^{\mu h(n)}$$

Solution to Representative $O\Delta E$

- The time-marching methods, given by Eqs. 8 to 10, rewritten

$$[E - (1 + \lambda h)]u_n = hae^{\mu hn} \tag{17}$$

$$[(1 - \lambda h)E - 1]u_n = h \cdot Eae^{\mu hn} \tag{18}$$

$$\begin{bmatrix} E & -(1+\lambda h) \\ -\frac{1}{2}(1+\lambda h)E & E - \frac{1}{2} \end{bmatrix} \begin{bmatrix} \tilde{u} \\ u \end{bmatrix}_n = h \begin{bmatrix} 1 \\ \frac{1}{2}E \end{bmatrix} ae^{\mu hn} \tag{19}$$

- Subsets of the *operational form* of the representative OΔE

$$\boxed{P(E)u_n = Q(E) \cdot ae^{\mu hn}} \tag{20}$$

Predictor-Corrector:Matrix Form $O\Delta E$

- Starting with Eq.10 and using E

$$
\begin{aligned}
E\tilde{u}_n - (1+\lambda h)u_n &= ahe^{\mu hn} \\
-\frac{1}{2}(1+\lambda h)E\tilde{u}_n + Eu_n - \frac{1}{2}u_n &= \frac{1}{2}Eahe^{\mu h(n)}
\end{aligned}
$$

$$
\begin{bmatrix} E & -(1+\lambda h) \\ -\frac{1}{2}(1+\lambda h)E & E-\frac{1}{2} \end{bmatrix} \begin{bmatrix} \tilde{u} \\ u \end{bmatrix}_n = h \begin{bmatrix} 1 \\ \frac{1}{2}E \end{bmatrix} ae^{\mu hn}
$$

General Solution to $O\Delta E$

- General solution for $\boxed{P(E)u_n = Q(E) \cdot ae^{\mu hn}}$

$$u_n = \sum_{k=1}^{K} c_k (\sigma_k)^n + ae^{\mu hn} \cdot \frac{Q(e^{\mu h})}{P(e^{\mu h})} \tag{21}$$

- $P(E)$: *characteristic polynomial*, $Q(E)$: *particular polynomial*
- σ_k are the K roots of the characteristic polynomial, $P(\sigma) = 0$.
- Coupled $O\Delta E$'s such as the Predictor-Corrector, Eq. 19
  - Determinants used to form $P(E)$ and $Q(E)$
  - The ratio $Q(E)/P(E)$ can be found by Cramer's rule.

Examples of Solutions: $O\Delta E$

- Euler Explicit: Eq. 17, we have

$$\begin{aligned} P(E) &= E - 1 - \lambda h \\ Q(E) &= h \end{aligned} \tag{22}$$

$$u_n = c_1(1+\lambda h)^n + ae^{\mu hn} \cdot \frac{h}{e^{\mu h} - 1 - \lambda h}$$

- Implicit Euler method, Eq. 18, we have

$$\begin{aligned} P(E) &= (1-\lambda h)E - 1 \\ Q(E) &= hE \end{aligned} \tag{23}$$

$$u_n = c_1\left(\frac{1}{1-\lambda h}\right)^n + ae^{\mu hn} \cdot \frac{he^{\mu h}}{(1-\lambda h)e^{\mu h} - 1}$$

- Coupled predictor-corrector equations, Eq. 19,
  - Solve for the final family u_n
  - Intermediate family $\tilde{u}$, not used in general
- Using Determinants for $P(E)$ and $Q(E)$

$$
\begin{aligned}
P(E) &= \det \begin{bmatrix} E & -(1+\lambda h) \\ -\frac{1}{2}(1+\lambda h)E & E-\frac{1}{2} \end{bmatrix} \\
&= E\left(E - 1 - \lambda h - \frac{1}{2}\lambda^2 h^2\right)
\end{aligned}
$$

$$
\begin{aligned}
Q(E) &= \det \begin{bmatrix} E & h \\ -\frac{1}{2}(1+\lambda h)E & \frac{1}{2}hE \end{bmatrix} \\
&= \frac{1}{2}hE(E + 1 + \lambda h)
\end{aligned}
$$

- The σ-root is found from

$$P(\sigma) = \sigma\left(\sigma - 1 - \lambda h - \frac{1}{2}\lambda^2 h^2\right) = 0$$

- One nontrivial root, ($\sigma = 0$ is trivial root)

$$\begin{aligned} u_n &= c_1\left(1 + \lambda h + \frac{1}{2}\lambda^2 h^2\right)^n + \\ & \quad a e^{\mu h n} \cdot \frac{\frac{1}{2} h\left(e^{\mu h} + 1 + \lambda h\right)}{e^{\mu h} - 1 - \lambda h - \frac{1}{2}\lambda^2 h^2} \end{aligned} \tag{24}$$

Establishing the $\sigma - \lambda$ Relation

- Introduced to two basic kinds of roots
  - λ-roots: eigenvalues of the A, defined by space differencing the original PDE
  - σ-roots: roots of the characteristic polynomial in a representative OΔE
- $\sigma - \lambda$ relationship: used to identify many of the essential properties of a time-march method.
- Solution to the ODE

$$\begin{aligned}\vec{u}(t) &= c_1\left(e^{\lambda_1 h}\right)^n \vec{x}_1 + \cdots + c_m\left(e^{\lambda_m h}\right)^n \vec{x}_m + \cdots \\ &+ c_M\left(e^{\lambda_M h}\right)^n \vec{x}_M \;+\; P.S.\end{aligned} \tag{25}$$

- Explicit Euler λ-root given by $\sigma = 1 + \lambda h$.

- The solution for $O\Delta E$

$$\begin{aligned}\vec{u}_n &= c_1(\sigma_1)^n\,\vec{x}_1 + \cdots + c_m(\sigma_m)^n\,\vec{x}_m + \cdots \\ &+ c_M(\sigma_M)^n\,\vec{x}_M \;+\; P.S. \end{aligned} \tag{26}$$

where the c_m and the $\vec{x}_m$ in the two equations are identical and $\sigma_m = (1 + \lambda_m h)$.

- Correspondence between σ_m and $e^{\lambda_m h}$.

- $e^{\lambda h}$ can be expressed in terms of the series

$$e^{\lambda h} = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \frac{1}{6}\lambda^3 h^3 + \cdots + \frac{1}{n!}\lambda^n h^n + \cdots$$

- The truncated expansion $\sigma = 1 + \lambda h$ approximates $e^{\lambda h}$
  - Define $er_\lambda = e^{\lambda h} - \sigma = O(\lambda^2 h^2)$.
  - $O\Delta E$ solution is for u_n
  - Typically define error for a derivative, e.g. er_t
  - Define Order of accuracy p for $O\Delta E$ as: $O(h^p) \equiv \frac{er_\lambda}{h}$
  - Euler explicit $O\Delta E$: $er_\lambda = O(h)$, a first order method.

Leapfrog $O\Delta E$

- Leapfrog method:

$$u_{n+1} \quad = u_{n-1} + 2hu'_n \tag{27}$$

- Characteristic polynomial

$$P(E) = E^2 - 2\lambda hE - 1$$

leads to

$$\sigma_m^2 - 2\lambda_m h\sigma_m - 1 = 0 \tag{28}$$

- Each λ produces two σ-roots

$$\sigma_m^{\pm} = \lambda_m h \pm \sqrt{1 + \lambda_m^2 h^2}$$

- For one of these we find

$$\begin{aligned}\sigma_m^+ &= \lambda_m h + \sqrt{1+\lambda_m^2 h^2} \\ &= 1 + \lambda_m h + \frac{1}{2}\lambda_m^2 h^2 - \frac{1}{8}\lambda_m^4 h^4 + \cdots \end{aligned} \tag{29}$$

- Approximation to $e^{\lambda_m h}$ with an error $O(\lambda^3 h^3)$.
- Therefore: $er_\lambda = O(h^2)$, a second order method.
- The other root, $\lambda_m h - \sqrt{1+\lambda_m^2 h^2}$, is a spurious root.

Principal and Spurious Roots

- Depending on the $\sigma - \lambda$ relation

Application of time-marching method to the equations in a coupled system of linear ODE's always produces one σ-root for every λ-root satisfying

$$\sigma = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \cdots + \frac{1}{k!}\lambda^k h^k + O\left(h^{k+1}\right)$$

where k is the order of the time-marching method.

  - There could be multiple σ roots
  - One is always the principal, $\sigma_1(h, \lambda)$
  - Note: $\sigma_1(h = 0, \lambda) = 1.0$, consistent with $e^{h\lambda} = 1, h = 0$
  - All other roots are spurious, typically inaccurate, and hopefully stable and small

Accuracy Measures of Time-Marching Methods

- Two broad categories of errors used to derive and evaluate time-marching methods.
  - Error made in each time step, This is a *local* error.
  - Such as that found from a Taylor table analysis, used as the basis for establishing the order of a method.
  - Error determined at the end of a given event, *global* error,
  - Covers a specific interval of time composed of many time steps.
  - Useful for comparing methods

- Taylor Series analysis is a very limited tool for finding the more subtle properties of a numerical time-marching method. For example, it is of no use in:
  - finding spurious roots.
  - evaluating numerical stability and separating the errors in phase and amplitude.
  - analyzing the particular solution of predictor-corrector combinations.
  - finding the global error.

Comparison of Exact ODE and $O\Delta E$ Error

- Exact solution to the representative ODE:

$$u(nh) = c\left(e^{\lambda h}\right)^n + \frac{a\left(e^{(\mu h)}\right)^n}{\mu - \lambda} \tag{30}$$

- Solution to the representative OΔE's, including only the contribution from the principal root:

$$u_n = c_1(\sigma_1)^n + ae^{\mu hn} \cdot \frac{Q(e^{\mu h})}{P(e^{\mu h})} \tag{31}$$

Error Measures for $O\Delta E$'s

- Transient error
  - All time-marching methods produce a principal σ-root for every λ-root that exists in a set of linear ODE's.
  - Compare the unsteady part of Eq.30, $e^{\lambda h}$
  - With the unsteady part of Eq.31, σ
  - Define, $\boxed{er_\lambda \equiv e^{\lambda h} - \sigma_1}$
  - With the Order of accuracy defined as $O(h^p) \equiv \frac{er_\lambda}{h}$
  - Or the term in the expansion of $e^{\lambda h}$ which matches the last term of er_λ .

- Amplitude and Phase Error
  - Assume λ eigenvalue is pure imaginary.
  - Equations governing periodic convection.
  - Let $\lambda = i\omega$ where ω is real representing a frequency.
  - Numerical method produces a principal σ-root: complex
  - Expressible in the form

$$\sigma_1 = \sigma_r + i\sigma_i \approx e^{i\omega h} \tag{32}$$

  - The local error in amplitude: deviation of $|\sigma_1|$ from unity

$$\boxed{er_a = 1 - |\sigma_1| = 1 - \sqrt{(\sigma_1)_r^2 + (\sigma_1)_i^2}}$$

  - Local error in phase can be defined as

$$\boxed{er_\omega \equiv \omega h - \tan^{-1}\left[(\sigma_1)_i/(\sigma_1)_r)\right]} \tag{33}$$

– Amplitude and phase errors are important measures of the suitability of time-marching methods for convection and wave propagation phenomena.

- Local Accuracy of the Particular Solution (er_μ)
  – Compare the particular solution of the ODE with that for the OΔE.

$$P.S._{(ODE)} = ae^{\mu t} \cdot \frac{1}{(\mu - \lambda)}$$

and

$$P.S._{(O\Delta E)} = ae^{\mu t} \cdot \frac{Q(e^{\mu h})}{P(e^{\mu h})}$$

  – Measure of the *local* error in the particular solution: introduce the definition

$$er_\mu \equiv h\left\{\frac{P.S._{(O\Delta E)}}{P.S._{(ODE)}} - 1\right\} \tag{34}$$

– Multiplication by h converts the error from a global measure to a local one, so that the order of er_λ and er_μ are consistent.

– Determine the leading error term, Eq. 34 in terms of the characteristic and particular polynomials as

$$\boxed{er_\mu = \frac{c_o}{\mu - \lambda} \cdot \left\{ (\mu - \lambda) Q\left(e^{\mu h}\right) - P\left(e^{\mu h}\right) \right\}} \tag{35}$$

– Expanded in a Taylor series, where

$$c_o = \lim_{h \to 0} \frac{h(\mu - \lambda)}{P\left(e^{\mu h}\right)}$$

The value of c_o is a method-dependent constant that is often equal to one.

– Algebra involved in finding the order of er_μ is quite tedious.

– An illustration of this is given in the section on Runge-Kutta methods.

Global Accuracy

- To compute some time-accurate phenomenon over a fixed interval of time using a constant time step.
- Let T be the fixed time of the event and h be the chosen step size.
- Then the required number of time steps, is N, $T = Nh$
  - Global error in the transient

$$Er_\lambda \equiv e^{\lambda T} - (\sigma_1(\lambda h))^N \tag{36}$$

  - Global error in amplitude and phase

$$Er_a = 1 - \left(\sqrt{(\sigma_1)_r^2 + (\sigma_1)_i^2} \right)^N \tag{37}$$

$$\begin{aligned} Er_\omega &\equiv N\left[\omega h - \tan^{-1}\left(\frac{(\sigma_1)_i}{(\sigma_1)_r}\right)\right] \\ &= \omega T - N\tan^{-1}\left[(\sigma_1)_i/(\sigma_1)_r\right] \end{aligned} \tag{38}$$

– Global error in the particular solution

$$Er_\mu \equiv (\mu - \lambda)\frac{Q\left(e^{\mu h}\right)}{P(e^{\mu h})} - 1$$

Linear Multistep Methods

The Linear Multistep Methods (LMM's) are probably the most natural extension to time marching of the space differencing schemes.

$$\sum_{k=1-K}^{1} \alpha_k u_{n+k} = h \sum_{k=1-K}^{1} \beta_k u'_{n+k}$$

Applying the representative ODE, $u' = \lambda u + ae^{\mu t}$, the characteristic polynominals $P(E)$ and $Q(E)$ are:

Linear Multistep Methods

$$\left[\left(\sum_{k=1-K}^{1} \alpha_k E^k\right) - \left(\sum_{k=1-K}^{1} \beta_k E^k\right) h\lambda\right] u_n = h\left(\sum_{k=1-K}^{1} \beta_k E^k\right) a e^{\mu h n}$$

$$[P(E)]\, u_n = Q(E) a e^{\mu h n}$$

Consistency requires that $\sigma \to 1$ as $h \to 0$ which is met if

$$\sum_k \alpha_k = 0 \quad \text{and} \quad \sum_k \beta_k = \sum_k (K + k - 1)\alpha_k$$

"Normalization" results in $\sum_k \beta_k = 1$

Families of Linear Multistep Methods

- Adams-Moulton family

$$\alpha_1 = 1, \qquad \alpha_0 = -1, \qquad \alpha_k = 0, \qquad k = -1, -2, \cdots$$

- Adams-Bashforth family: same α's with constraint: $\beta_1 = 0$.
- Three-step Adams-Moulton method

$$u_{n+1} = u_n + h(\beta_1 u'_{n+1} + \beta_0 u'_n + \beta_{-1} u'_{n-1} + \beta_{-2} u'_{n-2})$$

Taylor tables can be used to find classes of second, third and fourth order methods.

Examples of Linear Multistep Methods

Explicit Methods

$$
\begin{aligned}
u_{n+1} &= u_n + hu'_n && \text{Euler} \\
u_{n+1} &= u_{n-1} + 2hu'_n && \text{Leapfrog} \\
u_{n+1} &= u_n + \tfrac{1}{2}h\big[3u'_n - u'_{n-1}\big] && \text{AB2} \\
u_{n+1} &= u_n + \tfrac{h}{12}\big[23u'_n - 16u'_{n-1} + 5u'_{n-2}\big] && \text{AB3}
\end{aligned}
$$

Examples of Linear Multistep Methods

Implicit Methods

$$
\begin{aligned}
u_{n+1} &= u_n + hu'_{n+1} && \text{Implicit Euler} \\
u_{n+1} &= u_n + \tfrac{1}{2}h\left[u'_n + u'_{n+1}\right] && \text{Trapezoidal (AM2)} \\
u_{n+1} &= \tfrac{1}{3}\left[4u_n - u_{n-1} + 2hu'_{n+1}\right] && \text{2nd-order Backward} \\
u_{n+1} &= u_n + \tfrac{h}{12}\left[5u'_{n+1} + 8u'_n - u'_{n-1}\right] && \text{AM3}
\end{aligned}
$$

Two-Step Linear Multistep Methods

- Most general scheme $(1+\xi)u_{n+1} = [(1+2\xi)u_n - \xi u_{n-1}] + h\,[\,\theta u'_{n+1} + (1-\theta+\varphi)u'_n - \varphi u'_{n-1}]$
- Examples:

θ	ξ	φ	Method	Order
0	0	0	Euler	1
1	0	0	Implicit Euler	1
1/2	0	0	Trapezoidal or AM2	2
1	1/2	0	2nd Order Backward	2
3/4	0	−1/4	Adams type	2
1/3	−1/2	−1/3	Lees	2
1/2	−1/2	−1/2	Two–step trapezoidal	2
5/9	−1/6	−2/9	A–contractive	2
0	−1/2	0	Leapfrog	2
0	0	1/2	AB2	2
0	−5/6	−1/3	Most accurate explicit	3
1/3	−1/6	0	Third–order implicit	3
5/12	0	1/12	AM3	3
1/6	−1/2	−1/6	Milne	4

- Both er_μ and er_λ are reduced to $0(h^3)$ if $\varphi = \xi - \theta + \frac{1}{2}$
- The class of all 3rd-order methods $\xi = 2\theta - \frac{5}{6}$
- Unique fourth-order method is found by setting $\theta = -\varphi = -\xi/3 = \frac{1}{6}$.

Predictor-Corrector Methods

- Predictor-corrector methods are composed of sequences of linear multistep methods.
- Simple one-predictor, one-corrector scheme

$$\begin{aligned}\tilde{u}_{n+\alpha} &= u_n + \alpha h u'_n \\ u_{n+1} &= u_n + h\big[\beta \tilde{u}'_{n+\alpha} + \gamma u'_n\big]\end{aligned}$$

- α, β and γ are arbitrary parameters.

$$\begin{aligned}P(E) &= E^\alpha \cdot \big[E - 1 - (\gamma + \beta)\lambda h - \alpha\beta\lambda^2 h^2\big] \\ Q(E) &= E^\alpha \cdot h \cdot [\beta E^\alpha + \gamma + \alpha\beta\lambda h]\end{aligned}$$

- Second-order accuracy: *both* er_λ and er_μ must be $O(h^3)$.
- Leads to: $\gamma + \beta = 1 \quad ; \quad \alpha\beta = \frac{1}{2}$
- Second-order accurate predictor-corrector sequence for any α

$$\begin{aligned} \tilde{u}_{n+\alpha} &= u_n + \alpha h u'_n \\ u_{n+1} &= u_n + \frac{1}{2} h \left[\left(\frac{1}{\alpha} \right) \tilde{u}'_{n+\alpha} + \left(\frac{2\alpha - 1}{\alpha} \right) u'_n \right] \end{aligned}$$

Predictor-Corrector Methods: Examples

- The Adams-Bashforth-Moulton sequence for $k = 3$

$$\begin{aligned} \tilde{u}_{n+1} &= u_n + \frac{1}{2}h\big[3u'_n - u'_{n-1}\big] \\ u_{n+1} &= u_n + \frac{h}{12}\big[5\tilde{u}'_{n+1} + 8u'_n - u'_{n-1}\big] \end{aligned}$$

- The Gazdag method

$$\begin{aligned} \tilde{u}_{n+1} &= u_n + \frac{1}{2}h\big[3\tilde{u}'_n - \tilde{u}'_{n-1}\big] \\ u_{n+1} &= u_n + \frac{1}{2}h\big[\tilde{u}'_n + \tilde{u}'_{n+1}\big] \end{aligned}$$

- The Burstein method $\alpha = 1/2$ is

$$\begin{aligned} \tilde{u}_{n+1/2} &= u_n + \frac{1}{2} h u'_n \\ u_{n+1} &= u_n + h \tilde{u}'_{n+1/2} \end{aligned}$$

- MacCormack's method

$$\begin{aligned} \tilde{u}_{n+1} &= u_n + h u'_n \\ u_{n+1} &= \frac{1}{2} [u_n + \tilde{u}_{n+1} + h \tilde{u}'_{n+1}] \end{aligned}$$

Runge-Kutta Methods

- Runge-Kutta method of order k: principal σ-root is given by

$$\sigma = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \cdots + \frac{1}{k!}\lambda^k h^k$$

- To ensure kth order accuracy: $er_\mu = O(h^{k+1})$
- General RK(N) scheme

$$\begin{aligned}
\widehat{u}_{n+\alpha} = u_n &\quad + \quad \beta h u'_n \\
\tilde{u}_{n+\alpha_1} = u_n &\quad + \quad \beta_1 h u'_n + \gamma_1 h \widehat{u}'_{n+\alpha} \\
\overline{u}_{n+\alpha_2} = u_n &\quad + \quad \beta_2 h u'_n + \gamma_2 h \widehat{u}'_{n+\alpha} + \delta_2 h \tilde{u}'_{n+\alpha_1} \\
u_{n+1} = u_n &\quad + \quad \mu_1 h u'_n + \mu_2 h \widehat{u}'_{n+\alpha} + \mu_3 h \tilde{u}'_{n+\alpha_1} \\
&\qquad\qquad + \mu_4 h \overline{u}'_{n+\alpha_2}
\end{aligned}$$

Runge-Kutta Methods

- Total of 13 free parameters,where the choices for the time samplings, α, α_1, and α_2, are not arbitrary.

$$\begin{aligned} \alpha &= \beta \\ \alpha_1 &= \beta_1 + \gamma_1 \\ \alpha_2 &= \beta_2 + \gamma_2 + \delta_2 \end{aligned}$$

- Ten (10) free parameters remain to obtain various levels of accuracy, $er_\lambda, er_a, er_\omega, er_\mu$

Runge-Kutta Methods

- Finding $P(E)$ and $Q(E)$ and then eliminating the β's results in the four conditions

$$
\begin{aligned}
\mu_1 + \mu_2 + \mu_3 + \mu_4 &= 1 && (1)\\
\mu_2\alpha + \mu_3\alpha_1 + \mu_4\alpha_2 &= 1/2 && (2)\\
\mu_3\alpha\gamma_1 + \mu_4(\alpha\gamma_2 + \alpha_1\delta_2) &= 1/6 && (3)\\
\mu_4\alpha\gamma_1\delta_2 &= 1/24 && (4)
\end{aligned}
$$

- Guarantee that the five terms in σ exactly match the first 5 terms in the expansion of $e^{\lambda h}$.

- To satisfy the condition that $er_\mu = O(h^5)$

$$\mu_2\alpha^2 + \mu_3\alpha_1^2 + \mu_4\alpha_2^2 = 1/3 \quad (3)$$

$$\mu_2\alpha^3 + \mu_3\alpha_1^3 + \mu_4\alpha_2^3 = 1/4 \quad (4)$$

$$\mu_3\alpha^2\gamma_1 + \mu_4(\alpha^2\gamma_2 + \alpha_1^2\delta_2) = 1/12 \quad (4)$$

$$\mu_3\alpha\alpha_1\gamma_1 + \mu_4\alpha_2(\alpha\gamma_2 + \alpha_1\delta_2) = 1/8 \quad (4)$$

- Gives 8 equations for 10 unknowns.

RK4 Method

- Storage requirements and work estimates allow for a variety of choices for the remaining 2 parameters.
- "Standard" 4^{th} order Runge-Kutta method expressed in predictor-corrector form

$$\begin{aligned}
\widehat{u}_{n+1/2} &= u_n + \frac{1}{2} h u'_n \\
\tilde{u}_{n+1/2} &= u_n + \frac{1}{2} h \widehat{u}'_{n+1/2} \\
\overline{u}_{n+1} &= u_n + h \tilde{u}'_{n+1/2} \\
u_{n+1} &= u_n + \frac{1}{6} h \left[u'_n + 2\left(\widehat{u}'_{n+1/2} + \tilde{u}'_{n+1/2} \right) + \overline{u}'_{n+1} \right]
\end{aligned}$$

Implementation of Implicit Methods

- There are various trade-offs which must be considered in selecting a method for a specific application.
  - Representative ODE, $u' = \lambda u + ae^{\mu t}$

$$(1 - \lambda h)u_{n+1} - u_n = he^{\mu h} \cdot ae^{\mu hn}$$

  - Solving for u_{n+1} gives

$$u_{n+1} = \frac{1}{1 - \lambda h}(u_n + he^{\mu h} \cdot ae^{\mu hn}) \tag{39}$$

  - This calculation requires a division.

Implicit Euler For Coupled System

- Implicit Euler applied to $\vec{u}' = A\vec{u} - \vec{f}(t)$
- The equivalent to Eq. 39 is

$$(I - hA)\vec{u}_{n+1} - \vec{u}_n = -h\vec{f}(t+h) \tag{40}$$

$$\vec{u}_{n+1} = (I - hA)^{-1}[\vec{u}_n - h\vec{f}(t+h)] \tag{41}$$

- The inverse is not actually performed, but rather we solve Eq. 40 as a linear system of equations.

Example

- The system of equations which must be solved is tridiagonal (e.g., for biconvection, $A = -aB_p(-1, 0, 1)/2\Delta x$)
- Its solution is inexpensive in 1D,
- For multidimensions the bandwidth can be very large.
- Various techniques are used to make the solution process more efficient.

Application to Nonlinear Equations

- Consider the general *nonlinear* scalar ODE given by

$$\frac{du}{dt} = F(u,t) \tag{42}$$

- Implicit Euler method:

$$u_{n+1} = u_n + hF(u_{n+1}, t_{n+1}) \tag{43}$$

- Nonlinear difference equation.
- Requires complicated non-linear solution process for u_{n+1}

  – Example, nonlinear ODE:

$$\frac{du}{dt} + \frac{1}{2}u^2 = 0 \tag{44}$$

– Solved using implicit Euler time marching

$$u_{n+1} + h\frac{1}{2}u_{n+1}^2 = u_n \tag{45}$$

– Requires a nontrivial method to solve for u_{n+1}.

- Linearization to produce a solvable method

- Think in terms of small perturbations from a reference state

Local Linearization for Scalar Equations

- Expanding $F(u,t)$ about some reference point in time.
- Reference value t_n, the dependent variable u_n.
- A Taylor series expansion about these reference quantities

$$F(u,t) = F(u_n,t_n) + \left(\frac{\partial F}{\partial u}\right)_n (u-u_n) + \left(\frac{\partial F}{\partial t}\right)_n (t-t_n)$$
$$+\frac{1}{2}\left(\frac{\partial^2 F}{\partial u^2}\right)_n (u-u_n)^2 + \left(\frac{\partial^2 F}{\partial u \partial t}\right)_n (u-u_n)(t-t_n)$$
$$+\frac{1}{2}\left(\frac{\partial^2 F}{\partial t^2}\right)_n (t-t_n)^2 + \cdots \tag{46}$$

- Expansion of $u(t)$ in terms of the independent variable t is

$$u(t) = u_n + (t-t_n)\left(\frac{\partial u}{\partial t}\right)_n + \frac{1}{2}(t-t_n)^2\left(\frac{\partial^2 u}{\partial t^2}\right)_n + \cdots \tag{47}$$

- Assuming t is within h of t_n, both $(t - t_n)^k$ and $(u - u_n)^k$ are $O(h^k)$, and Eq. 46 can be written

$$F(u,t) = F_n + \left(\frac{\partial F}{\partial u}\right)_n (u - u_n) + \left(\frac{\partial F}{\partial t}\right)_n (t - t_n) + O(h^2) \qquad (48)$$

- This represents a second-order-accurate, locally-linear approximation to $F(u,t)$ that is valid in the vicinity of the reference station t_n

- Locally time-linear representationof $\frac{du}{dt} = F(u,t)$

$$\frac{du}{dt} = \left(\frac{\partial F}{\partial u}\right)_n u + \left(F_n - \left(\frac{\partial F}{\partial u}\right)_n u_n\right) + \left(\frac{\partial F}{\partial t}\right)_n (t - t_n) + O(h^2)$$

Implementation of the Trapezoidal Method

- The trapezoidal method is given by

$$u_{n+1} = u_n + \frac{1}{2}h[F_{n+1} + F_n] + hO(h^2) \tag{49}$$

- Note $hO(h^2)$: emphasizes second order accurate of method
- Using Eq. 48 to evaluate $F_{n+1} = F(u_{n+1}, t_{n+1})$

$$u_{n+1} = u_n + \frac{1}{2}h\left[F_n + \left(\frac{\partial F}{\partial u}\right)_n (u_{n+1} - u_n)\right. \tag{50}$$

$$\left. + h\left(\frac{\partial F}{\partial t}\right)_n + O(h^2) + F_n\right]$$

$$+ hO(h^2) \tag{51}$$

- Note that the $O(h^2)$ term within the brackets (which is due to the local linearization) is multiplied by h and therefore is the same order as the $hO(h^2)$ error from the trapezoidal method.

- The *local linearization updated at each time step has not reduced the order of accuracy* of a second-order time-marching process.
- Assuming the $F(u)$ is not an explicit function of time, t
- Reordering of the terms in Eq. 50

$$\left[1 - \frac{1}{2}h\left(\frac{\partial F}{\partial u}\right)_n\right]\Delta u_n = hF_n \tag{52}$$

- The delta form.

Implementation of the Implicit Euler Method

- First-order implicit Euler method can be written

$$u_{n+1} = u_n + hF_{n+1} \tag{53}$$

- Introduce Eq. 49, rearrange terms

$$\left[1 - h\left(\frac{\partial F}{\partial u}\right)_n\right]\Delta u_n = hF_n \tag{54}$$

- The only difference between the implementation of the trapezoidal method and the implicit Euler method is the factor of $\frac{1}{2}$ in the brackets of the left side of Eqs. 52 and 54.

Newton's Method

- Consider the limit $h \to \infty$ of Eq. 54 obtained by dividing both sides by h and setting $1/h = 0$. There results

$$-\left(\frac{\partial F}{\partial u}\right)_n \Delta u_n = F_n \tag{55}$$

or

$$u_{n+1} = u_n - \left[\left(\frac{\partial F}{\partial u}\right)_n\right]^{-1} F_n \tag{56}$$

- Newton method for finding the roots of the nonlinear $F(u) = 0$.
- Implicit Euler is just under-relaxed Newton's Method